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HEURISTICS FOR GLOBAL OPTIMIZATION OF CONSTRAINED NONLINEAR PROGRAMS

by

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We consider the problem of finding the global solution to non-convex nonlinear programs which may have local solutions distinct from the global solution. Several heuristic methods are proposed. The advantage and disadvantages of heuristic methods as compared with algorithmic methods are discussed.

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Definition: A solution $x^* \in F$ is a local optimal solution for NLP if there exists a neighborhood N of x^* such that $f(x^*) \leq f(x)$ for all $x \in F \cap N$.

If f, g_i are all convex functions, then we call NLP a convex program, and the following properties hold:

1. The feasible region F is a convex set.
2. Any local optimal solution to NLP is also a global optimal solution.

For general, possibly nonconvex f, g_i we can no longer guarantee these properties. In particular,

1. The feasible region is not necessarily a convex set, in fact it is not even necessarily a connected set.

2. There may exist local optimal solutions which are not global optimal.

Most of the well known nonlinear optimization algorithms will terminate when a local solution has been found and are not able to determine whether or not this solution is also global. Algorithms for extending local optimizers to find global solutions have recently been developed (see [9] for a summary of several methods). They can conveniently be divided into two classes, heuristic methods and algorithmic methods.

Algorithmic methods are guaranteed to converge to a global optimal solution (perhaps only as the limit of an infinite sequence of operations). Also, and perhaps more important, the computations are organized in such a way that when the global solution is found, the algorithm can eventually recognize that the solution is, in fact, global and will thus terminate.

The best examples of algorithmic methods are the various versions of the branch and bound algorithm as developed by Falk and Soland[2], Falk [3], Soland [11], and Beale & Tomlin [1].

Heuristic methods, on the other hand, can be characterized as techniques which are plausible approaches to global optimization, but for which no convergence proof is known. Many heuristics can guarantee arbitrarily high probabilities of attaining the global optimum (if sufficiently large numbers of computations are done), but the critical difference is that a heuristic can never proclaim with certainty that the global solution has been found. Some examples of heuristic methods are found in Hesse [7], Hartman [5,6] and Opacic [10].

Algorithmic methods concentrate on gathering the information needed to prove that the best solution found is, in fact, global, while heuristic methods concentrate on rapidly attaining good solutions and perhaps some degree of confidence that the best solution found is a global optimal solution. Particularly relevant to this last goal is the work by Liau, Hartley, and Sielken [8] in which statistical confidence regions for the global solution are developed.

Algorithmic methods are known only for certain classes of problems. In particular the branch and bound methods mentioned above require that NLP be a separable program. Heuristics are, in general, not so restricted, although particular computational schemes may apply only to particular problem types.

The primary advantage of algorithmic methods over heuristics lies in the positive guarantee of global optimality which algorithmic methods

can provide. The disadvantages are first, that algorithmic methods may be too slow to converge so that, in practice, the guarantee of global optimality is meaningless; and second, that special problem structures are required. The preferred method probably depends on the particular problem to be solved. There is not sufficient computational experience available at this time to formulate general rules of choice.

II. COMPONENTS FOR HEURISTIC GLOBAL OPTIMIZERS

In this section we discuss some basic building blocks which can be combined in various ways to develop heuristic global optimizers for solving the nonconvex NLP problem. In particular, the following structural components will be considered.

A) Search methods for finding constrained local solutions to NLP.

B) Procedures for obtaining new starting points for repeated application of the local search methods.

C) Procedures for moving away from one local solution in an attempt to find a better one.

D) Procedures for early termination of local searches which appear to be converging to local solutions which are already known.

Combination of these components to form heuristic global optimizers will be considered in section III.

A. Local Optimizers. Methods for finding constrained local optimal solutions to nonlinear programs are well developed. In particular penalty function methods would seem particularly relevant to the purpose of nonconvex optimization since they do not depend upon any convexity properties of the constraint functions or feasible region. We distinguish two classes of methods:

A1. Interior penalty functions (also known as barrier functions) the best known example is the SUMT function [4].

$$P(x,r) = f(x) + r \sum_{i=1}^{m} \frac{1}{b_i - g_i(x)}, \quad r > 0$$

Interior methods require an initial feasible x.

A2. Exterior penalty functions such as

$$Q(x,r) = f(x) + r \sum_{i=1}^{m} [\min(0, b_i - g_i(x))]^2$$

Exterior methods do not require initial feasible solutions. It should be noted however, that for nonconvex problems there is no guarantee that the exterior penalty function method will converge to a feasible solution, so we must be prepared to correct for this problem if it occurs.

B. Starting Points. Perhaps the oldest proposal for global optimization is to repeatedly apply a local optimizer starting each local optimization from a different initial point. Comparisons of several procedures for effectively selecting starting points for unconstrained global optimization can be found in [5] and [6], and similar procedures are worthy of consideration for the constrained NLP. The constrained case is more difficult since if we wish to use an interior penalty method for the local optimizer, then the starting point must be in the interior of the feasible region F. Several possible methods are indicated below:

B1. Sample x from a uniform random distribution over the set

$$S^0 = \{x \mid L_j < x_j < U_j; \quad j = 1, \ldots, n\}.$$

If also

$$x \in R^0 = \{x \mid g_i(x) < b_i; \quad i = 1, \ldots, m\}$$

then use x as a new starting point for local optimization. Otherwise repeat the process, continuing to sample $x \varepsilon S^0$ until $x \varepsilon R^0$ is found. The probability of finding a feasible starting point at any trial is the ratio of the volume of $S^0 \cap R^0$ to the volume of S^0 which is generally not known. Note, however, that if the problem contains an equality constraint, then the volume of R^0 is zero and this method is not appropriate.

B2. Sample $x \varepsilon S^0$ randomly. If also $x \varepsilon R^0$ then x is a new starting point. If $x \notin R^0$, let

$$I1 = \{i \mid g_i(x) \geq b_i, \quad i = 1, \ldots, m\}$$

and

$$I2 = \{i \mid g_i(x) < b_i, \quad i = 1, \ldots, m\}$$

Then formulate the "feasibility finding problem"

$$\text{FFP} \quad \min \sum_{i \varepsilon I1} g_i(x)$$

$$\text{st. } g_i(x) \leq b_i \quad i \varepsilon I2$$

$$L_j \leq x_j \leq U_j \quad j = 1, \ldots, n$$

and use an interior penalty function method to solve it. If a violated constraint (in I1) becomes satisfied during the solution process it is moved to I2 and the process continues until either a feasible starting point is found, or a minimum to FFP is found but is not in R^0. In the latter case a new $x \varepsilon S^0$ is sampled and the process repeats. This

feasibility finding problem is due to Fiacco & McCormick [4].

B3. If exterior penalty functions are to be used for NLP, then any $x \in E^n$ is suitable as a starting point, but it would seem reasonable to restrict the choice to a random selection of $x \in S$. Unfortunately, there is no guarantee that convergence to a feasible point will occur since the exterior penalty function may be unbounded over E^n. Since exterior penalty functions generally converge to a point which is slightly infeasible it may be difficult to decide when the pathological behavior is occurring.

B4. A better use of exterior penalties might be in a mixed interior - exterior function. Select $x \in S^0$ randomly. Let I1 and I2 be defined as above, and formulate the mixed interior - exterior penalty function problem:

$$\min_{x \in E^n} f(x) + r \sum_{i \in I2} \frac{1}{b_i - g_i(x)} + r \sum_{i \in I1} [\min(0, b_i - g_i(x)]^2 + r \sum_{j=1}^{n} \left(\frac{1}{U_j - x_j} + \frac{1}{x_j - L_j}\right)$$

Minimization of this penalty function will maintain feasibility for the constraints in I2 and the upper and lower bounds on x_j while attempting to converge to feasibility for the violated constraints in I1.

B5. Each of the above methods B1 - B4 selects random points $x \in S^0$ without regard to where previous random points were selected. In [5] a method is developed which keeps track of the previously selected starting points and the trajectories from these starting points to the local optimal solutions found during previous searches. The new $x \in S^0$ can then be selected to avoid researching portions of S which have already been searched.

This modification could be applied to any of B1 - B4 as presented above. Evidence in [5] for the unconstrained problem indicates that this modification may significantly improve the efficiency of global search procedures. Details of the procedure can be found in [5].

C. Leaving a Local Solution. Once a local solution has been found by the local search algorithm, we face the problem of how to continue the search to find another hopefully better local solution. One procedure is to select a new starting point as in B1 - B5 hoping that a local search from the new point will converge to a new local solution.

A more systematic procedure is to move away from the local solution keeping track of the penalty function value. Initially this value will increase, (since we are leaving a local minimum). If it subsequently begins to decrease then the chances are good that we have moved into the "region of attraction" of a different local minimum. Starting the local optimization algorithm at this point should then lead to a new local optimal solution to NLP. Two versions of this idea are:

C1. Move away from the local solution along some feasible direction d (one which points into the feasible region F). This involves potential difficulties if the boundary of F is reached before the penalty function value decreases. Perhaps a better idea is the following:

C2. Suppose $P(x,r)$ is the penalty function (interior, exterior, or mixed) which has been minimized to find the current local solution x^*. Add a new constraint

$$g_0(x) = \sum_{j=1}^{n} (x_j - x_j^*)^2 \geq b_0^2$$

to the NLP problem. This constraint defines a hypersphere of radius b_0 centered at x^* whose interior now becomes infeasible, hence excluding the local solution x^*. Let

$$P^*(x,r,b_0) = P(x,r) + r\,[\min(0,g_0(x)-b_0)]^2$$

be the penalty function resulting from augmenting the original $P(x,r)$ with an exterior term for the new constraint. Let $x^*(b_0)$ be the solution to $\min_x P^*(x,r,b_0)$. Gradually increasing the radius b_0 of the exclusion constraint will tend to drive $x^*(b_0)$ away from the local solution x^*. Continue to increase b_0 until either,

a) $P(x^*(b_0),r)$ increases and then eventually decreases. Then continue to minimize $P(x,r)$ starting from this new point, or

b) no feasible $x^*(b_0)$ can be found. Then procedure C_2 has failed.

Hyperspheric exclusion constraints have been previously considered by others (notably Hesse [7]) as devices for excluding local solutions. In these cases, however, the exclusion constraints have been retained for the subsequent local searches thus permanently excluding the local solution x^* from feasibility in the subsequent searches. This necessitates searching for the smallest possible radius b_0 to avoid the chance of also inadvertently excluding the global solution from further consideration. For our purposes the exclusion constraints are only temporary devices for moving away from a local solution. The risk of subsequently revisiting this same local solution is deemed preferable to the risk of permanently excluding the global solution.

D. Termination of Local Searches. If procedures such as those referenced in B5 are used to keep track of previously found local minima and, perhaps, the search trajectories leading to them, then subsequent local searches can be terminated prior to convergence if they seem to be repeating work which has already been done.

D1. The simplest procedure is to maintain a record of the local minima found so far. If a subsequent search comes within a tolerance distance δ of one of these solutions, then terminate that search. This procedure can save considerable effort even if δ is quite small since the bulk of the work with most local searches seems to be expended obtaining convergence close to the solution rather than arriving in the vicinity of the solution.

D2. If also a record of past search trajectories is maintained, then we can terminate any subsequent search which comes closer than a tolerance ε to one of these trajectories. This involves substantially more bookkeeping and testing than D1, but computational experience for the unconstrained problem in [5] indicates that it can be a desirable procedure.

III. AN OUTLINE FOR SOME HEURISTIC GLOBAL OPTIMIZATION METHODS.

The components described in the previous section can be combined to form heuristic global optimization methods. One possible combination is indicated in the flow chart of figure 1.

Specifying the procedure to be used in each block (e.g., B1, B2, B3, B4, or B5) will determine a specific optimization method which fits this general pattern. The best choice is probably problem dependent in a fashion which is not now understood. We hope to do further computational experiments in the future to improve our ability to specify the particular global search heuristic which is most likely to be successful for a given problem.

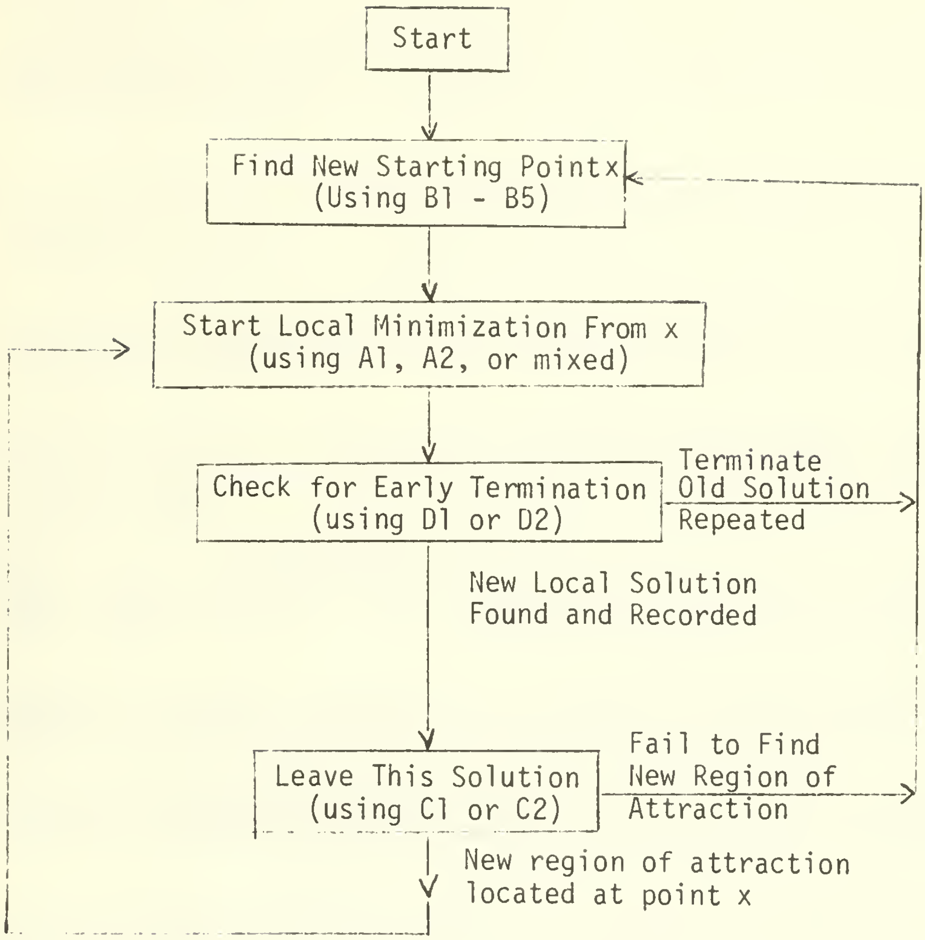

FIGURE 1

Flow Chart for Heuristic Global Optimizer

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